The Study of Ion-Pairing and Ion-Solvation in Lithium Battery Electrolytes by Soft X-ray Absorption/Emission Spectroscopy

Abstract

Recently there have been successful efforts to understand the hydrogen bonding in water and ice, and the ion-solvation interactions in aqueous media by using O *1s* X-ray absorption spectroscopy (XAS) and resonant X-ray emission spectroscopy (XES) combined with *ab-initio* Hartree-Fock and Density Functional Theory (DFT) simulations. Such methods have not yet been extended to study the structure of aprotic solvents and the ion-solvation in non-aqueous electrolytes. We propose a systematic approach to the study of ion-pairing and ion solvation in prototypical aprotic solvents, e.g. ethers such as polyethylene oxide (PEO), and alkyl carbonates such as propylene carbonate (PC), by a combination of C and O *1s* XAS, XES, aided by DFT simulations of the structures and the X-ray absorption/emission spectra. The lithium salts are selected to have anions that vary systematically in both size and orbital character so that the contribution from anion solvation to ion-pairing can be separated from the contribution of Li ion solvation and cation-anion binding. The results will be used to interpret trends in conductivity and the behavior of the same electrolytes in lithium batteries, e.g. Li insertion reactions.